Carboxin 5234-68-4 | DTXSID0023951

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Model	I)ata
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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 3.83 days

Global applicability domain: Inside

Local applicability domain index: 4.39e-01

Confidence level: 8.62e-01

Nearest Neighbors from the Training Set

Image not found

1H-Indene, 2-methyl-Measured: 12.5 Predicted: 2.48 Image not found

5-Methylindan Measured: 4.93 Predicted: 2.25 Image not found

4-Methylindan Measured: 4.93 Predicted: 2.31

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3-Methylindene Measured: 12.5 Predicted: 2.76 Image not found

9-Ethyl-9H-fluorene Measured: 2330 Predicted: N/A